Dimethyl decanedioate

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Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 60.7

Global applicability domain: Inside

Local applicability domain index: 3.27e-01

Confidence level: 5.89e-01

Nearest Neighbors from the Training Set

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Dibutyl phthalate Measured: 166 Predicted: 14.2

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Methyl o-benzoylbenzoate

Measured: 14.1 Predicted: 9.17

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1,3-Diphenylguanidine

Measured: 20.0 Predicted: 9.15

Image not found

Phoxim
Measured: 813
Predicted: 52.4

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Benzyl butyl phthalate Measured: 16.2 Predicted: 19.6